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Published in:
Book of Abstracts. DTU's Sustain Conference 2015

Publication date:
2015

Document Version
Publisher's PDF, also known as Version of record

New free Danish online (Q)SAR predictions database with >600,000 substances

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(Q)SARs are models that can predict properties, e.g. toxicity, for chemical substances solely based on their structure. Since 2005 the Danish (Q)SAR Database has been freely available on the Internet. It is a tool that allows single chemical substance profiling and screenings based on predicted hazard information. The database is also included in the OECD (Q)SAR Application Toolbox, which is a free software application to fill information gaps needed for assessing the hazards of chemicals. The free software is used worldwide by regulators and industry. A lot of progress in (Q)SAR model development, application and documentation has been made since the publication in 2005.

A new and completely rebuild online (Q)SAR predictions database was therefore published in November 2015 at http://qsar.food.dtu.dk. The number of chemicals in the database has been expanded from 185,000 to >600,000. As far as possible all organic single constituent substances that were pre-registered under REACH have been included in the new structure set. The new Danish (Q)SAR Database includes estimates from more than 200 (Q)SAR models covering a wide range of hazardous properties relevant for human health and the environment such as acute toxicity to rat, mouse, fish, daphnia and algae, as well as many physical-chemical and environmental fate properties, skin irritation, sensitization, genotoxicity, cancer, endocrine activity and reproductive toxicity. In agreement with software vendors, (Q)SAR predictions for 600,000 substances from commercial and free software (CASE Ultra, Leadscope PDM, SciQSAR, ACD/Tox Suite and EPI Suite) are included in the database.

The database is one of the most comprehensive freely available (Q)SAR tools for substance evaluations and large-scale screenings. The online interface to the database allows for advanced combination of searches as well as sorting functions on chemical similarity. Negotiations are underway with the OECD to integrate the new database with the OECD (Q)SAR Application Toolbox. The database was developed by the DTU National Food Institute in cooperation and with financial support from the Danish Environmental Protection Agency, the Nordic Council of Ministers and the European Chemicals Agency (ECHA).